

Three-leg Antiferromagnetic Heisenberg Ladder with Frustrated Boundary Condition; Ground State Properties

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The antiferromagnetic Heisenberg spin systems on the three-leg ladder are investigated. Periodic boundary condition is imposed in the rung direction. The system has an excitation gap for all antiferromagnetic inter-chain coupling ($J_{\perp} > 0$). The estimated gap for the strong coupling limit ($J_{\perp}/J_1 \rightarrow \infty$) is $0.28J_1$. Although the interaction is homogeneous and only nearest-neighbor, the ground states of the system are dimerized and break the translational symmetry in the thermodynamic limit. Introducing the next-nearest neighbor coupling (J_2), we can see that the system is solved exactly. The ground state wave function is completely dimer-ordered. Using density matrix renormalization group algorithm, we show numerically that the original model ($J_2 = 0$) has the same nature with the exactly solvable model. The ground state properties of the ladder with a higher odd number of legs are also discussed.

KEYWORDS: odd-legs ladder, dimerization, frustration

§1. Introduction

Nowadays there is much attention for quantum ladder systems.¹⁾ One of the reason is that the ladder systems are the first step from one-dimensional toward two-dimensional.^{2,3,4)} The other reason is caused by the advance of experimental techniques. Many materials which seem to be ladders are found and investigated extensively.^{5,6,7)} The antiferromagnetic spin systems are among the simplest many body systems which include strong quantum effect. From the analysis using the $O(3)$ non-linear σ model,⁸⁾ antiferromagnetic spin ladders with an even number of legs are expected to have an excitation gap. In this case, as for the existence of an excitation gap, the system is not sensitive to the boundary condition perpendicular to the chain. For the two-leg $S = 1/2$ spin ladder there are many works and it is confirmed that there is an excitation gap.^{9,10,11)} On the other hand, in the case of a ladder with an odd number of legs, the topology is important.¹²⁾ (For the fermion systems, there are works about the importance of the topology,^{4,13)} which treat the repulsive Hubbard ladder with weak electron-electron coupling limit using field theoretical argument.) The odd-leg ladders with open boundary condition in the rung direction (we will call it as open ladder) has no frustrated interaction. These can be considered effectively as $S = 1/2$ antiferromagnetic Heisenberg chain (AFHC)^{8,14)}. On the other hand, periodic boundary condition in the rung direction (cylindrical ladder) causes frustrated interaction. The frustration changes the situation dramatically. There is also attention for the dimer-ordered phase. We know the $S = 1/2$ AFHC is unstable for the dimer interaction. The model becomes gapful as the dimer interaction is inserted.¹⁵⁾ However the model breaks the translational invariance a priori. The Majumdar-Ghosh model is one of the typical models with which ground states are frustration induced dimer-ordered and have translational invariance in the finite size system.¹⁶⁾ In this paper we show another example of the model with frustration induced dimer-ordered ground states. We consider following antiferromagnetic Heisenberg Hamiltonian,

$$\mathcal{H}_1 = J_1 \sum_{n=1}^{N'} \sum_i H_{n,n}^{i,i+1} + J_\perp \sum_{n=1}^{N'} \sum_i H_{n,n+1}^{i,i} \quad (1)$$

where $H_{n,m}^{i,j} = \mathbf{S}_{n,i} \cdot \mathbf{S}_{m,j}$ and $\mathbf{S}_{n,i}$ is $S = 1/2$ $SU(2)$ spin operator. We concentrate on the condition, $J_1, J_\perp \geq 0$. Subscripts and superscripts n, m and i, j represent the site number in the rung direction and the chain direction respectively. The number of legs and the number of sites along the chain are N and L respectively. (The total number of sites is NL .) For the open ladder we set $N' = N - 1$ and for the cylindrical ladder we set $N' = N$ and $N + 1 \equiv 1$. The boundary condition

along the chain direction is appropriately treated and denoted periodic boundary condition and open one as PBC and OBC respectively. In almost all part of this paper (except for §4), we will consider the three-leg ladder $N = 3$. We add the next-nearest neighbor interaction,

$$\mathcal{H}_2 = J_2 \sum_{n=1}^{N'} \sum_i H_{n,n}^{i,i+2}, \quad (2)$$

to see the system more explicitly. (See below.) Then the total Hamiltonian is $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$. In the case of $J_\perp = 0$, we know the model well for a few parameter points. The model with $(J_1, J_\perp, J_2) = (J_1, 0, 0)$, which is exactly solved by Bethe Ansatz,¹⁷⁾ has no frustrated interaction and ground state is proved to be spin singlet by Marshall-Lieb-Mattis Theorem. The model has gapless excitation and belongs to the universality class of the level-1 $SU(2)$ WZW model in the low energy limit. We know the long-distance asymptotic behavior of correlation functions, for example, spin-spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ and dimer-dimer correlation function $\langle (\mathbf{S}_0 \cdot \mathbf{S}_1)(\mathbf{S}_r \cdot \mathbf{S}_{r+1}) \rangle - \langle \mathbf{S}_0 \cdot \mathbf{S}_1 \rangle \langle \mathbf{S}_r \cdot \mathbf{S}_{r+1} \rangle$ decay as $(-1)^r/r$ (up to logarithmic corrections¹⁸⁾). For the other parameter point $(J_1, 0, J_1/2)$, which is the so-called Majumder-Ghosh model,¹⁶⁾ the ground states are well-known in the sense that we exactly know the wave function. The ground state wave function is dimerized and written down by direct products of two-site spin-singlet. Therefore the ground states are doubly degenerate and break the translational invariance. The existence of the excitation gap is exactly proved.¹⁹⁾ By the bosonization approach, we know that the perturbation by J_2 is marginal. (Whether the operator is relevant or irrelevant is determined by the sign of the initial coupling constant. In the decoupled chains case ($J_\perp = 0$), the transition point is $J_2 = 0.2411 \dots$ ²⁰⁾) On the other hand, perturbation by J_\perp is strongly relevant compared with that of J_2 .^{12, 21)} Therefore we expect that the total Hamiltonian with $J_\perp > 0$ is essentially represented by the effective Hamiltonian with $J_\perp/J_1 \rightarrow \infty$.

Our strategy to investigate the model is as follows. First, we introduce the effective Hamiltonian in the strong coupling limit ($J_\perp \rightarrow \infty$), which is the fixed point of the renormalization group. We add the next-nearest neighbor coupling (J_2) to the model. Then we show the model with special coupling ($J_2/J_1 = 1/2, J_\perp/J_1 \rightarrow \infty$) is solved exactly. (In the sense that we can construct the exact ground state wave function.) Using the density matrix renormalization group (DMRG) algorithm introduced by White,²²⁾ we see the original model ($J_2 = 0$ and $0 < J_\perp/J_1 \leq \infty$) has the same nature with the exactly solved model by calculating the expectation value of the local Hamiltonian operator. We also confirm that there is no transition between

$0 \leq J_2/J_1 \leq 1/2$ through seeing no level crossing in low-energy excitation spectra by numerical exact diagonalization. The estimation of the excitation gap for various value of J_\perp is also showed. In §4 we shortly mention the cylindrical ladders with a higher odd number of legs. For general odd number of legs N , we construct effective Hamiltonian in the strong coupling limit, which has the same form with the case of $N = 3$.

§2. Strong-Coupling Effective Hamiltonian

We first consider the strong coupling limit ($J_\perp \rightarrow \infty$) of the three-leg ladder. The reason is as following. In bosonization language (weak coupling analysis), the inter-chain coupling causes the relevant operator through the staggered part of the spin operator,^{12, 21)} so generally the system is expected to flow into the strong coupling limit in renormalization processes, i.e. the strong coupling limit is the fixed point of the renormalization flow. In the case of the open ladder with $J_1 = 0$ (which is understood as $J_\perp = \infty$), the ground state of each rung is a doublet. Then the effective Hamiltonian of the original Hamiltonian (1) in the strong coupling limit is represented by,

$$\mathcal{H}_{\text{eff}} = J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (3)$$

Therefore, in this limit, the system can be described by $S = 1/2$ AFHC as noted in the introduction. The model has no excitation gap, power-law decaying spin-spin correlation, and it is classified into the same universality of level-1 $SU(2)$ WZW model.²³⁾ The vanishing excitation gap is proved by Affleck and Lieb.²⁴⁾ On the other hand, in the case of the cylindrical ladder, we cannot prove the existence of a gapless excitation by the theorem because the uniqueness of the ground state is not proved. The ground state of the three-site ring is four-fold degenerate, these states are,

$$\begin{aligned} |\uparrow L\rangle &= \frac{1}{\sqrt{3}} \left(|\uparrow\uparrow\downarrow\rangle + \omega |\uparrow\downarrow\uparrow\rangle + \omega^{-1} |\downarrow\uparrow\uparrow\rangle \right), \\ |\downarrow L\rangle &= \frac{1}{\sqrt{3}} \left(|\downarrow\downarrow\uparrow\rangle + \omega |\downarrow\uparrow\downarrow\rangle + \omega^{-1} |\uparrow\downarrow\downarrow\rangle \right), \\ |\uparrow R\rangle &= \frac{1}{\sqrt{3}} \left(|\uparrow\uparrow\downarrow\rangle + \omega^{-1} |\uparrow\downarrow\uparrow\rangle + \omega |\downarrow\uparrow\uparrow\rangle \right), \\ |\downarrow R\rangle &= \frac{1}{\sqrt{3}} \left(|\downarrow\downarrow\uparrow\rangle + \omega^{-1} |\downarrow\uparrow\downarrow\rangle + \omega |\uparrow\downarrow\downarrow\rangle \right), \end{aligned}$$

where $\omega = \exp(\frac{2\pi i}{3})$. The indices L, R represent the momentum of the three site ring, $k = 2\pi/3$, and $-2\pi/3$ respectively. The four-fold degeneracy essentially distinguishes the cylindrical ladder from the open ladder. The other states have higher

energy of order J_\perp . Therefore in the strong coupling limit $J_\perp/J_1 \rightarrow \infty$, the effective Hamiltonian is,¹²⁾

$$\mathcal{H}_{\text{eff}} = \frac{J_1}{3} \sum_i H_{\text{eff}}^{i,i+1}(\alpha) \quad \text{with} \quad \alpha = 4. \quad (4)$$

where $H_{\text{eff}}^{i,i+1}(\alpha) = \mathbf{S}_i \cdot \mathbf{S}_{i+1} \left(1 + \alpha(\tau_i^+ \tau_{i+1}^- + \tau_i^- \tau_{i+1}^+)\right)$. Though we write α explicitly for convenience through this section, it should be considered as 4. The operators τ^\pm exchange indices L, R such as,

$$\begin{aligned} \tau^+ |\cdot L\rangle &= 0, & \tau^- |\cdot L\rangle &= |\cdot R\rangle, \\ \tau^+ |\cdot R\rangle &= |\cdot L\rangle, & \tau^- |\cdot R\rangle &= 0. \end{aligned}$$

(In these equations the dots represent \downarrow or \uparrow .) We define the diagonal operator τ^z which, with $\tau^x = (\tau^+ + \tau^-)/2$ and $\tau^y = (\tau^+ - \tau^-)/2i$, satisfies commutation relation of three generators of $SU(2)$.

For the two-site system, the ground state wave function of the Hamiltonian (4) is,

$$\begin{aligned} &|\uparrow L, \downarrow R\rangle - |\downarrow L, \uparrow R\rangle + |\uparrow R, \downarrow L\rangle - |\downarrow R, \uparrow L\rangle \\ &\equiv (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \cdot (|LR\rangle + |RL\rangle), \end{aligned} \quad (5)$$

the corresponding energy is $-\frac{1}{4}(1 + \alpha)J_1$. In the following, we write this wave function as, $\bullet \leftrightarrow \bullet$. The wave function (5) can be also written down in the three-leg ladder language. The wave function in the three-leg ladder is the sum of three terms which are $[1_1, 2_1] \otimes [1_2, 1_3] \otimes [2_2, 2_3]$ and ones translated in the rung direction i.e.,

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Here $[\cdot, \cdot]$ represents the two-site spin-singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. Of course the expression is not unique, we are able to write it in more complicated form with two site spin singlet states.

Next we add the next-nearest neighbor coupling (Hamiltonian \mathcal{H}_2). Then the total effective Hamiltonian is,

$$\mathcal{H}_{\text{eff}} = \frac{J_1}{3} \sum_i H_{\text{eff}}^{i,i+1}(\alpha) + \frac{J_2}{3} \sum_i H_{\text{eff}}^{i,i+2}(\alpha). \quad (6)$$

With special coupling $J_1 = 2J_2$, we find exact ground states as follows. Define the operator P ,

$$P_{i,i+1,i+2} = \frac{1}{2}(H_{\text{eff}}^{i,i+1}(\alpha) + H_{\text{eff}}^{i+1,i+2}(\alpha) + H_{\text{eff}}^{i,i+2}(\alpha)) + \frac{3}{8}(1 + \alpha). \quad (7)$$

Using this operator P the Hamiltonian (6) is represented by

$$\mathcal{H}_{\text{eff}} = \frac{J_1}{3} \sum_i (P_{i,i+1,i+2} - \frac{3}{8}(1 + \alpha)). \quad (8)$$

The operator $P_{i,i+1,i+2}$ is small dimensional, we, therefore, easily proved the semi-positive definiteness of it. The number of eigenvectors with the eigenvalue zero is 12, and these eigenvectors are represented in the following three types,

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i.e. P is the linear combination of projection operators with positive coefficients, which projects out these three states. The situation is closely similar to the case of the Majumdar-Ghosh model. The difference is that P is not represented by a single projection operator. Then the two states,

$$\begin{array}{lcl} |\psi_1\rangle = & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet \\ |\psi_2\rangle = & \bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet\text{---}\bullet & \bullet \\ & 1 & & & & & & & L \end{array}$$

are, at least, among the ground states with energy $-\frac{1}{8}(1 + \alpha)LJ_1$. (For PBC case, the site 1 and L of the wave function $|\psi_2\rangle$ are connected by a line. For OBC case, $|\psi_2\rangle$ is degenerate because of the degrees of freedom of site 1 and L .) These ground states are evidently dimerized. In finite-size system with PBC we construct two ground states with the momentum 0 and π as $(|\psi_1\rangle + |\psi_2\rangle)/\sqrt{2}$ and $(|\psi_1\rangle - |\psi_2\rangle)/\sqrt{2}$. We also confirmed that only these two states are ground states by numerical exact diagonalization up to 12-site system. For the two ground states, obviously, correlation functions $\langle S_0^z S_r^z \rangle$ and $\langle \tau_0^z \tau_r^z \rangle$ have zero correlation except for the nearest neighbor. The wave function is site local, it strongly suggests the existence of the excitation gap. We, unfortunately, have not found the exact proof of it.

In the next section we perform the numerical calculation using DMRG algorithm. The DMRG prefers OBC to PBC. Therefore we prepare the appropriate order parameter for the discussion of the above models, which should show whether the ground state of the system is dimerized. Note that for the case of OBC, if we take the Hamiltonian as,

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= \frac{J_1}{3} \sum_{i=1}^{L-1} H_{\text{eff}}^{i,i+1}(\alpha) + \frac{J_1}{6} \sum_{i=1}^{L-2} H_{\text{eff}}^{i,i+2}(\alpha) \\ &= \frac{J_1}{3} \sum_{i=1}^{L-2} (P_{i,i+1,i+2} - \frac{3}{8}(1+\alpha)) + \frac{J_1}{6} (H_{\text{eff}}^{1,2}(\alpha) + H_{\text{eff}}^{L-1,L}(\alpha)),\end{aligned}\quad (9)$$

the ground state is not degenerate for the finite-size system because of the last bracketed terms. $|\psi_2\rangle$ has higher energy than $|\psi_1\rangle$ with $\frac{1}{4}(1+\alpha)J_1$ for all finite system size. Define the local Hamiltonian operator,

$$H_{\text{local}}^{i,i+1} = H_{\text{eff}}^{i,i+1}(\alpha) - \frac{1}{L-1} \sum_{j=1}^{L-1} \langle H_{\text{eff}}^{j,j+1}(\alpha) \rangle. \quad (10)$$

In the three-leg ladder case, we replace $H_{\text{eff}}^{i,i+1}$ with $\sum_{n=1}^3 (H_{n,n}^{i,i+1} + H_{n,n+1}^{i,i} + H_{n,n+1}^{i+1,i+1})$. For the Hamiltonian (9), the expectation value of this operator apparently has long-range order, i.e.,

$$\langle H_{\text{local}}^{i,i+1} \rangle = (-1)^i \frac{3}{8} (1+\alpha),$$

where we assume $L \equiv 2 \pmod{4}$. Therefore non-vanishing expectation value of this operator toward the center of the system explicitly means that the system has dimerized ground state, and breaks the translational symmetry in the thermodynamic limit. On the other hand, in the case of the open ladder (effectively this model is considered as $S = 1/2$ AFHC with OBC), the expectation value of this operator is decaying as $(-1)^r/\sqrt{r}$ (up to logarithmic correction), where r is distance from the boundary. This is because the scaling dimension of the dominant part of the local Hamiltonian is one-half.

§3. Numerical Calculations

In this section we perform numerical calculations using DMRG algorithm to show the original three-leg ladder system has the same nature with the exactly solvable model, such as a non-zero excitation gap, a finite correlation length of the spin-spin correlation function and a doubled unit cell of the ground state wave function. In the following calculations, we use the finite-size algorithm of DMRG which is necessary for the system with a large number of degrees of freedom in a single-site block. (The number of degrees of freedom for the three-leg ladder is $2^3 = 8$, and that for

the effective Hamiltonian is $2^2 = 4$.) We also show the result of $S = 1/2$ AFHC (effective Hamiltonian of the open ladder) or the open ladder for comparison. Note that $S = 1/2$ AFHC and the open ladders are expected to have power-law decaying correlation functions.

First we show the result of the effective Hamiltonian (4). In Fig. 1 we check the truncation-dependent accuracy by calculating triplet excitation gap ($S_{\text{total}}^z = 1, \tau_{\text{total}}^z = 0$) in the case of truncation numbers $m = 60$ and 80 for the finite-size algorithm. By the figure we can see that $m = 80$ for the finite-size algorithm is enough for the calculation. It looks also that there is an excitation gap. The inset is the data for $m = 80$ and the fitting function $0.277 + 0.276 \exp(-0.0387L)$. The extrapolated value of an excitation gap in the thermodynamic limit is $0.27(7)$. In Fig. 2 we plot the spin-spin and $\tau^z - \tau^z$ correlation functions for the system size 74 ($m = 80$). Both of them are exponentially decaying. The correlation length is estimated as $2.7(4)$. In Fig. 3 we show the expectation value of the local Hamiltonian operator (10). The figure shows that the expectation value is not decaying. This is the strong evidence to show that the ground state of the system is dimerized and breaks the translational symmetry in the thermodynamic limit. To be convinced more carefully that all the system with $0 \leq J_2/J_1 \leq 1/2$, $J_\perp \rightarrow \infty$ is in the same phase, we see the low energy spectra of the effective model with PBC by numerical exact diagonalization up to 12 sites (Fig. 4 shows 12 sites spectra for $J_2/J_1 = 0, 0.25$ and 0.5). There is no level crossing which supports no transition between $J_2/J_1 = 0$ and 0.5 . Secondly we show the result of the three-leg ladder. We pick up the typical value of $J_\perp = 1, 5$ and 10 and the system size is 22×3 . In Fig. 5 spin-spin correlation functions are plotted. They look like exponentially decaying. The correlation length tends to increase as J_\perp decreases. We also check the truncation error by comparing the spin-spin correlation functions for truncation number $m = 40, 60$ and 80 . (Inset of Fig. 5) On the other hand, the data for the open ladders are power-law decaying as expected showing the system is critical. We show the data for the expectation value of the local Hamiltonian operator in Fig. 6. These values do not decay, expressing long-range dimer-order. These results suggest that the cylindrical ladder is essentially represented by the strong coupling model (Hamiltonian(4)) as expected by the renormalization group analysis. On the other hand, for the open ladders the expected results showing that the systems belong to the universality class of level-1 $SU(2)$ WZW model are obtained. Finally in Fig. 7 we show the extrapolated values of the triplet excitation gap of the cylindrical ladder for typical values of J_\perp/J_1 using data up to 22×3 sites. The fitting function is deduced from the effective Hamiltonian

(Fig. 1), which is $a + b \exp(-cL)$, where a, b , and c are fitting constants.

§4. Higher Number of Odd Legs Cylindrical Ladders

In this section we comment on cylindrical ladders with a higher odd number of legs in the strong coupling limit ($J_\perp \rightarrow \infty$). The ground states of an odd-sites antiferromagnetic ring are four-fold degenerate. (Though there is no exact proof of it, we expect this from the exact numerical diagonalization of small system size and field theory for a large number of system size. See ref. 25.) We can derive the strong coupling effective Hamiltonian of the N -leg ($N = \text{odd}$) cylindrical ladder (See Appendix for derivation of it.) which is given as,

$$\mathcal{H}_{\text{eff}}^N = \frac{J_1}{N} \sum_i H_{\text{eff}}^{i,i+1}(\alpha). \quad (11)$$

Here α is positive and dependent on the number of legs N . For example 5-leg case $\alpha = 64/9$. To calculate analytically the N -dependence of α is too complicated for a higher number of legs. For small numbers of legs, however, we easily determine α numerically from the numerical exact diagonalization of system size $N \times 2$. In Fig. 8 we plot the extrapolated value of α for $N = 3, 5, 7, 9$ and 11 using data up to $J_\perp = 2048$. The figure shows that α increases as the number of legs increases. In Fig. 9, we plot the spin-spin correlation function and the local Hamiltonian operator with α corresponding to $N = 5$ and 7. The system size and truncation number are $L = 50$ and $m = 80$, respectively. These figures show that the effective models for cylindrical ladders of $N = 5, 7$ legs have dimerized ground states and it suggests that there is an excitation gap.

§5. Summary and Discussion

We study the ground state properties of the antiferromagnetic Heisenberg model on an odd number of legs cylindrical ladder. This model has frustrated interaction in the rung direction. The frustration induces the dimerization and the model has an excitation gap, that is different from the open ladder (which is with the open boundary condition in the rung direction.). The essential point distinguishing the cylindrical ladder from the open ladder seems to be the degeneracy of the ground state of odd-site antiferromagnetic Heisenberg chain i.e. the number of freedom of single site in the strong coupling effective Hamiltonian. First we consider the three-leg cylindrical ladder. We reduce the effective Hamiltonian (4) of the strong coupling limit ($J_\perp \rightarrow \infty$), which is expected to be the fixed point of the renormalization group treatment. We introduce the next-nearest neighbor coupling (J_2) for the effective Hamiltonian. For the model with special coupling ($J_1 = 2J_2$), we can construct the

exact ground state wave functions, which is direct products of two-site system wave function. This construction is closely analogous to Majumdar-Ghosh model. The wave function is apparently dimerized. The exactly solvable model is expected to have an excitation gap because the wave function is site-local. To confirm that the original system ($J_2=0$) has same nature with the exactly solvable model, we perform the numerical calculations using DMRG algorithm for the effective model and the three-leg cylindrical ladders. Adding to the spin-spin correlation function and triplet excitation gap, we calculate the expectation value of the local Hamiltonian operator which expresses the ground state being dimerized. The result shows that the three-leg cylindrical ladders are dimerized and essentially expressed by the strong coupling effective model.

Lastly we briefly study the cylindrical ladders with a higher odd number of legs. We can calculate the strong coupling effective Hamiltonian for the general number of legs, which is the same form with the three-leg ladder. The N -dependence is inserted into the parameter α . We have already known the exact solution for general α if we add the next-nearest neighbor interaction $J_2(=J_1/2)$. We expect the dimerization occurs for general N even in the case of $J_2=0$. We also confirm this expectation using DMRG calculations for small number of legs. We should comment on the ladder with a large odd number of legs. From the Fig. 8 we see that positive parameter α is monotonous as a function of N up to $N=11$, we, therefore, expect that α for large number of legs are between 4 and ∞ . It is likely from Fig. 9 that at least in the strong coupling limit the finite number of odd legs cylindrical ladder is dimerized in the ground state. The calculation in §4 is the strong coupling limiting case, therefore, in this study we cannot mention about the connection between 2-dimensional isotropic Heisenberg model (which has Neel order and gapless spin wave excitation) and the effective model studied here.

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Appendix: The Effective Hamiltonian for General N

In this Appendix, we derive the effective Hamiltonian (11) for general N . As denoted in §4, the ground states of odd-sites antiferromagnetic ring are four-fold degenerate (two doublets) and these two doublets have opposite sign of momentum i.e. these momenta are k and $-k$. We write these four states as $|\uparrow L\rangle, |\downarrow L\rangle, |\uparrow R\rangle$ and $|\downarrow R\rangle$. Here L and R represent the momentum k and $-k$ ($k \neq 0$), and we set $\omega = \exp(ik)$. Note that interchanging L and R corresponds to interchanging ω and ω^{-1} . Matrix elements of $S_{n,i}^z$ and $S_{n,i}^+$ in the restricted Hilbert space are

$$\begin{aligned} \langle \uparrow L | S_{n,i}^z | \uparrow L \rangle &= a_n, & \langle \uparrow R | S_{n,i}^z | \uparrow R \rangle &= a_n^*, \\ \langle \uparrow L | S_{n,i}^z | \uparrow R \rangle &= b_n, & \langle \uparrow R | S_{n,i}^z | \uparrow L \rangle &= b_n^*, \\ \langle \uparrow L | S_{n,i}^+ | \downarrow L \rangle &= c_n, & \langle \uparrow R | S_{n,i}^+ | \downarrow R \rangle &= c_n^*, \\ \langle \uparrow L | S_{n,i}^+ | \downarrow R \rangle &= d_n, & \langle \uparrow R | S_{n,i}^+ | \downarrow L \rangle &= d_n^*, \end{aligned}$$

where n is the site number of odd site ring and a^* represents the complex conjugate of a . It is obvious that interchanging \uparrow and \downarrow is interchanging the sign of a_n and b_n and setting $c_n = d_n = 0$. We set T is one-site shift operator for the n -direction, i.e. $T^m |\uparrow L\rangle = \omega^m |\uparrow L\rangle$ and $T^m |\uparrow R\rangle = \omega^{-m} |\uparrow R\rangle$. Then we conclude using the relation $T^m S_{n,i}^z T^{-m} = S_{n+m,i}^z$ that

$$a_n = a_1, \quad b_n = b_1 \omega^{-2(n-1)}, \quad c_n = c_1, \quad d_n = d_1 \omega^{-2(n-1)}. \quad (\text{A}\cdot 1)$$

The operator S_i^z of the effective Hamiltonian is the sum of $S_{n,i}^z$. Then using the relation eqs.(A-1) we know $a = 1/2N$. Setting the spin reversal operator P as $\prod_{n=1}^N 2S_{n,i}^x$, we can derive the relations,

$$c_1 = \langle \uparrow L | S_{1,i}^+ | \downarrow L \rangle = \langle \downarrow L | P S_{1,i}^+ P | \uparrow L \rangle = \langle \downarrow L | S_{1,i}^- | \uparrow L \rangle = c_1^*, \quad (\text{A}\cdot 2)$$

i.e. c_1 is also an real number. We also note that $\sum_{n=1}^N b_n^2 = \sum_{n=1}^N b_n = \sum_{n=1}^N d_n^2 = \sum_{n=1}^N d_n = 0$. Finally we obtain the effective Hamiltonian of the cylindrical ladder for general N ,

$$\begin{aligned} \mathcal{H}_{\text{eff}}^N = J_1 \sum_i \left\{ 4S_i^z S_{i+1}^z \sum_{n=1}^N \left(a_n^2 + |b_n|^2 (\tau_i^+ \tau_{i+1}^- + \tau_i^- \tau_{i+1}^+) \right) \right. \\ \left. + \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \sum_{n=1}^N \left(c_n^2 + |d_n|^2 (\tau_i^+ \tau_{i+1}^- + \tau_i^- \tau_{i+1}^+) \right) \right\}. \quad (\text{A}\cdot 3) \end{aligned}$$

In the derivation above, the $SU(2)$ symmetry of the each interaction $\mathbf{S}_{n,i} \cdot \mathbf{S}_{n,i+1}$ is preserved, so it should be that the effective Hamiltonian (A-3) also possesses the symmetry. This means that $4a_1^2 = c_1^2$ and $|b_1|^2/a_1^2 = |d_1|^2/c_1^2$. Then we reached the result (11) with $\alpha = |b_1|^2/a_1^2 (> 0)$.

We calculate α for $N = 5$ as follows. The ground states for 5-sites ring ($H = \sum_{n=1}^5 \mathbf{S}_{n,i} \cdot \mathbf{S}_{n+1,i}$) with energy $-\frac{1}{4}(2\sqrt{5} + 3)$ are

$$|\uparrow L\rangle = \frac{1}{\sqrt{|\beta_1|^2 + |\beta_2|^2}}(\beta_1|\text{I}_1\rangle + \beta_2|\text{II}_1\rangle),$$

where $\beta_1 = (\omega^{-1} + \omega^{-2})/2$, $\beta_2 = -(\omega^{-1} + \omega) - \frac{3}{2}$ and $\omega = \exp(\frac{2}{5}i\pi)$. The vectors $|\text{I}_1\rangle$ and $|\text{II}_1\rangle$ are

$$\begin{aligned} |\text{I}_1\rangle &= \frac{1}{\sqrt{5}} \left(|\uparrow\uparrow\uparrow\downarrow\downarrow\rangle + \omega|\uparrow\uparrow\downarrow\downarrow\uparrow\rangle + \omega^2|\uparrow\downarrow\downarrow\uparrow\uparrow\rangle + \omega^{-2}|\downarrow\downarrow\uparrow\uparrow\uparrow\rangle + \omega^{-1}|\downarrow\uparrow\uparrow\downarrow\downarrow\rangle \right) \\ |\text{II}_1\rangle &= \frac{1}{\sqrt{5}} \left(|\uparrow\downarrow\uparrow\downarrow\uparrow\rangle + \omega|\downarrow\uparrow\downarrow\uparrow\uparrow\rangle + \omega^2|\uparrow\downarrow\uparrow\uparrow\downarrow\rangle + \omega^{-2}|\downarrow\uparrow\downarrow\downarrow\uparrow\rangle + \omega^{-1}|\uparrow\uparrow\downarrow\uparrow\downarrow\rangle \right). \end{aligned}$$

Other three states $|\downarrow L\rangle$, $|\uparrow R\rangle$ and $|\downarrow R\rangle$ are produced by interchanging \uparrow and \downarrow or taking complex conjugate. After calculations we get,

$$b_1 = \frac{-2\omega^{-1} + 3\omega - 3\omega^2}{5(|\beta_1|^2 + |\beta_2|^2)}. \quad (\text{A}\cdot 4)$$

This leads to the result $\alpha = 64/9$.

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Figure captions

Fig. 1. The finite size triplet excitation gap for the effective Hamiltonian ($L = 74$). The data is for the truncation number $m = 60$ (\bigcirc) and 80 (\times). The inset is the data for $m = 80$ and the fitting function $0.277 + 0.276 \exp(-0.0387L)$.

Fig. 2. The correlation functions $(-1)^r \langle S_{L/2}^z S_{L/2+r}^z \rangle$ (\square) and $(-1)^r \langle \tau_{L/2}^z \tau_{L/2+r}^z \rangle$ ($+$) for the effective Hamiltonian with system size $L = 74$ and truncation number $m = 80$ are plotted in semi-log scale. The lines are for the guide to eyes ($1.58 \times 10^{-2} \exp(-r/2.74)$ and $3.74 \times 10^{-3} \exp(-r/2.74)$).

Fig. 3. The expectation value of the local Hamiltonian operator $(-1)^r \langle H_{\text{local}}^{r,r+1} \rangle$ (The symbol $+$, $1 \leq r \leq L/2$) is plotted in log-log scale for the effective Hamiltonian of the same L and m with Fig.2. The symbol \diamond is for $S = 1/2$ AFHC and the line is $0.20/\sqrt{r}$.

Fig. 4. The low-energy spectra for the effective Hamiltonian in the periodic boundary condition with $J_2/J_1 = 0, 0.25$ and 0.5 . The system size L is 12. x-axis is lattice momentum in unit $2\pi/L$. The symbols \square, \times , are spin-singlet with $\tau_{\text{total}}^z = 0$ and $\tau_{\text{total}}^z = 1$ (The blacked symbol represents lowest two spin-singlet with $\tau_{\text{total}}^z = 0$), the symbols \triangle, \bigcirc are spin-triplet with $\tau_{\text{total}}^z = 0$ and $\tau_{\text{total}}^z = 1$, respectively.

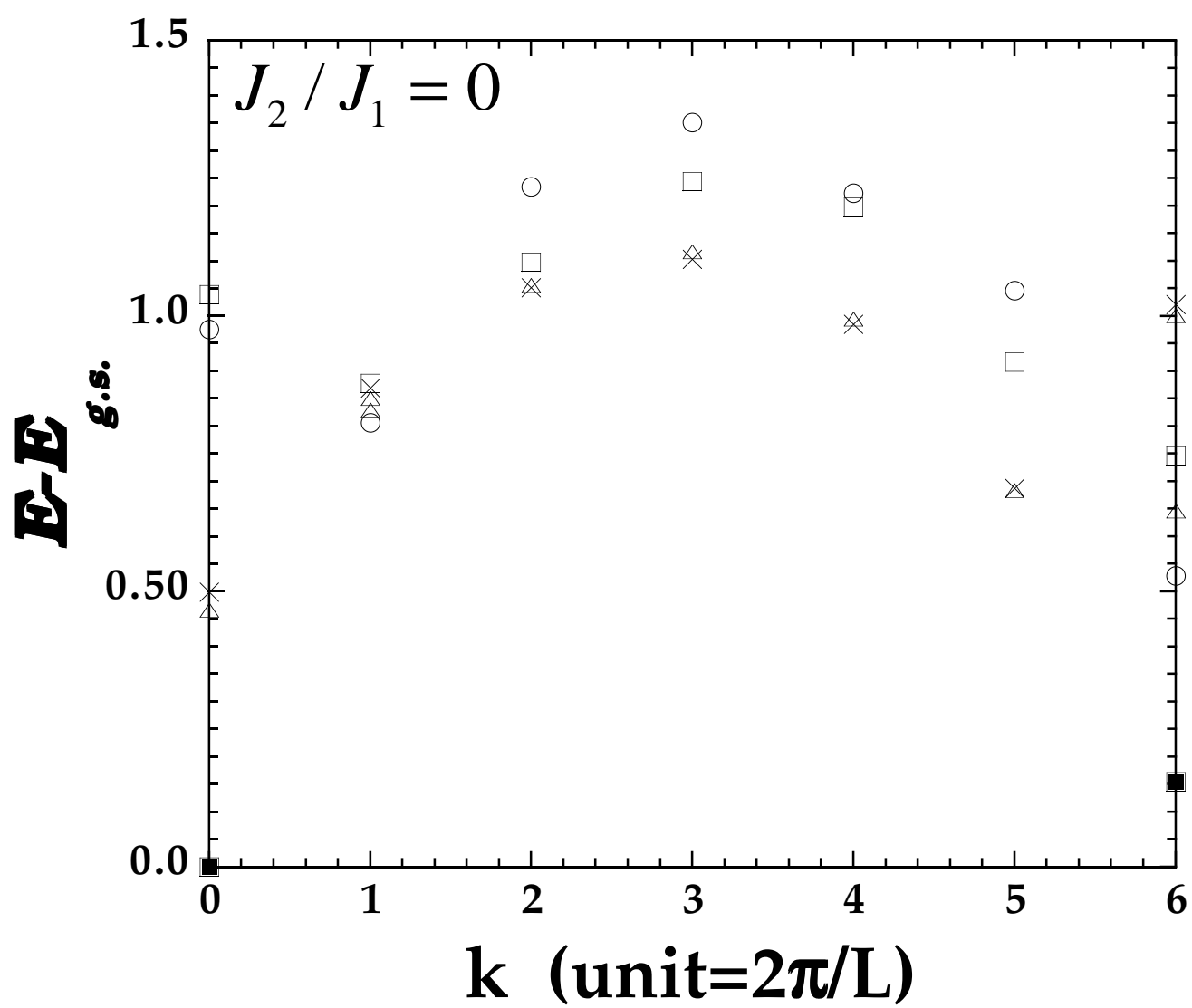
Fig. 5. The correlation function $(-1)^r \langle S_{L/2}^z S_{L/2+r}^z \rangle$ for the three-leg ladders. (We use semi-log scale for cylindrical ladders and log-log scale for open ladders.) The system size is 22×3 and truncation number $m = 60$. We choose typical J_\perp as 1 (\square), 5 (\triangle) and 10 (\times). The inset is the data for the cylindrical ladder with $J_\perp = 5$ with $m = 40(\times)$, $60(\triangle)$, and $80(\diamond)$, we can see $m = 60$ is enough for the calculation.

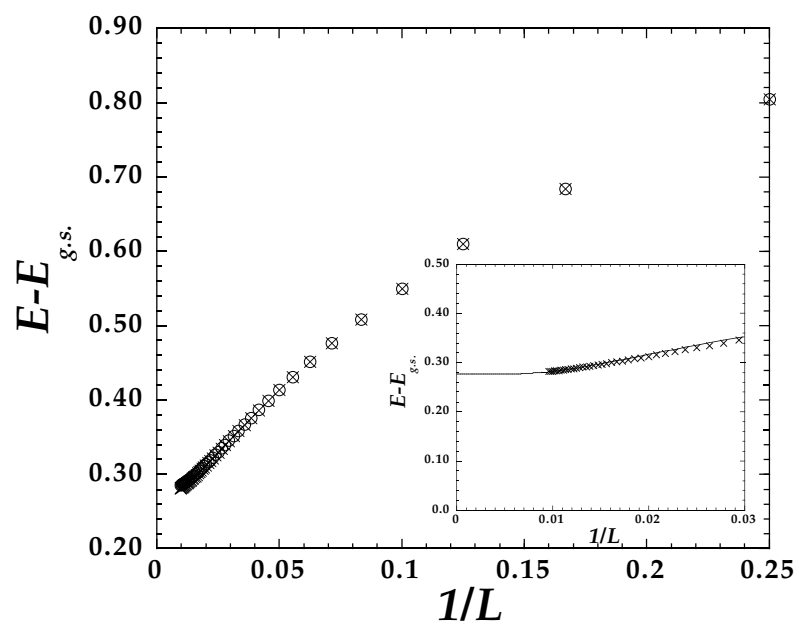
Fig. 6. The expectation value of local Hamiltonian operator $(-1)^r \langle H_{\text{local}}^{r,r+1} \rangle$ ($1 \leq r \leq L/2$) for three-leg open ladders (black) and cylindrical ladders (white) with $L = 22, N = 3$. (The symbols \diamond , \square and ∇ are for $J_\perp = 1, 5$ and 10 , respectively. The line $0.20/\sqrt{r}$ are guide to eyes.)

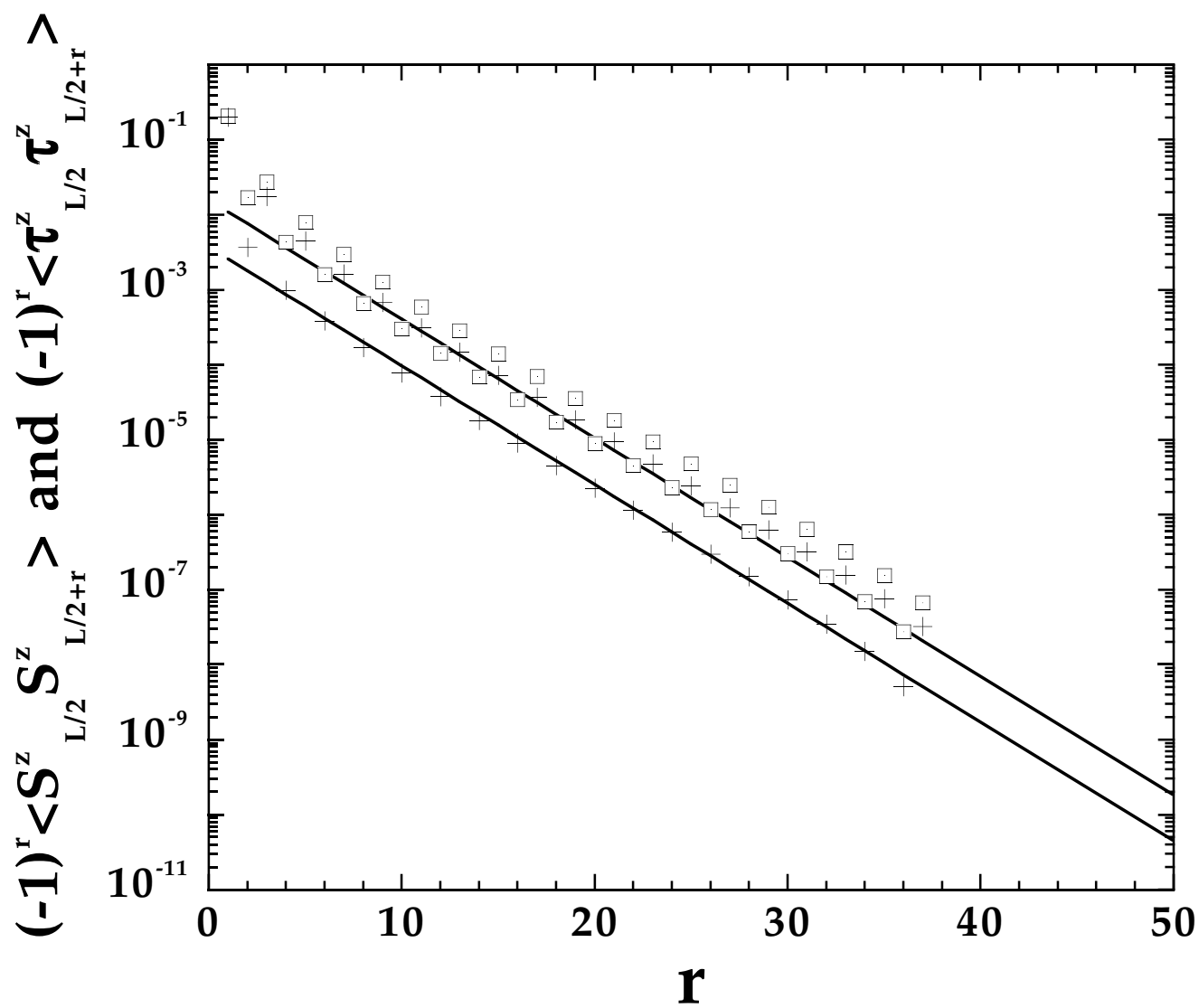
Fig. 7. The extrapolated value of the triplet excitation gap for the three-leg cylindrical ladders, using the data up to 22×3 with $m = 60$. The dotted line $(0.27(7))$ is the gap of the effective Hamiltonian($J_\perp \rightarrow \infty$).

Fig. 8. The extrapolated value of α for the higher number of legs cylindrical ladder using the data of the numerical exact diagonalization of $N \times 2$ sites.

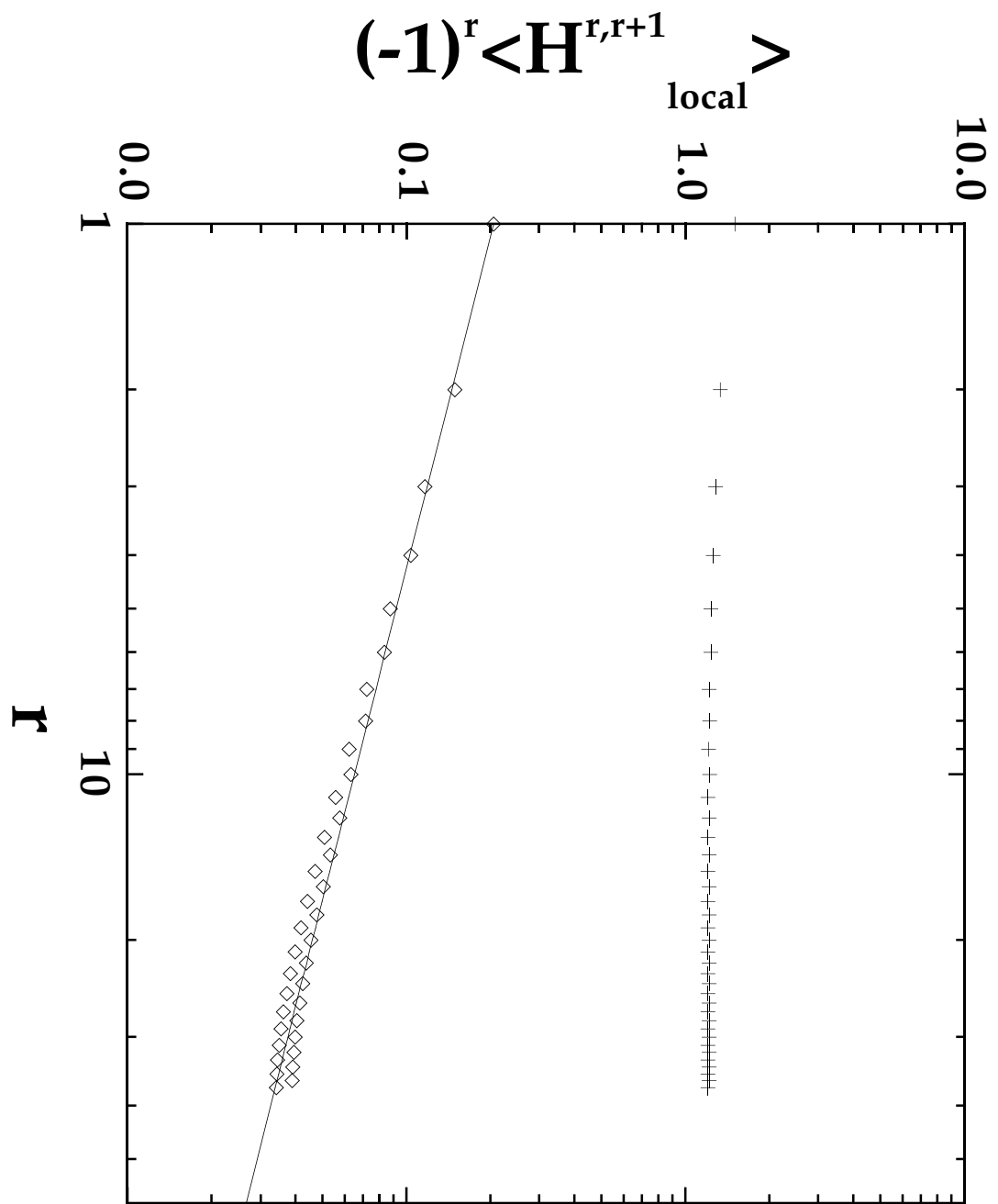
Fig. 9. The correlation function $(-1)^r \langle S_{L/2}^z S_{L/2+r}^z \rangle$ and the local Hamiltonian operator $(-1)^r \langle H_{\text{local}}^{r,r+1} \rangle$ ($1 \leq r \leq L/2$) of the effective Hamiltonian with $N = 3$ (\diamond), 5 (\square) and 7 (\triangle) are plotted in semi-log scale.

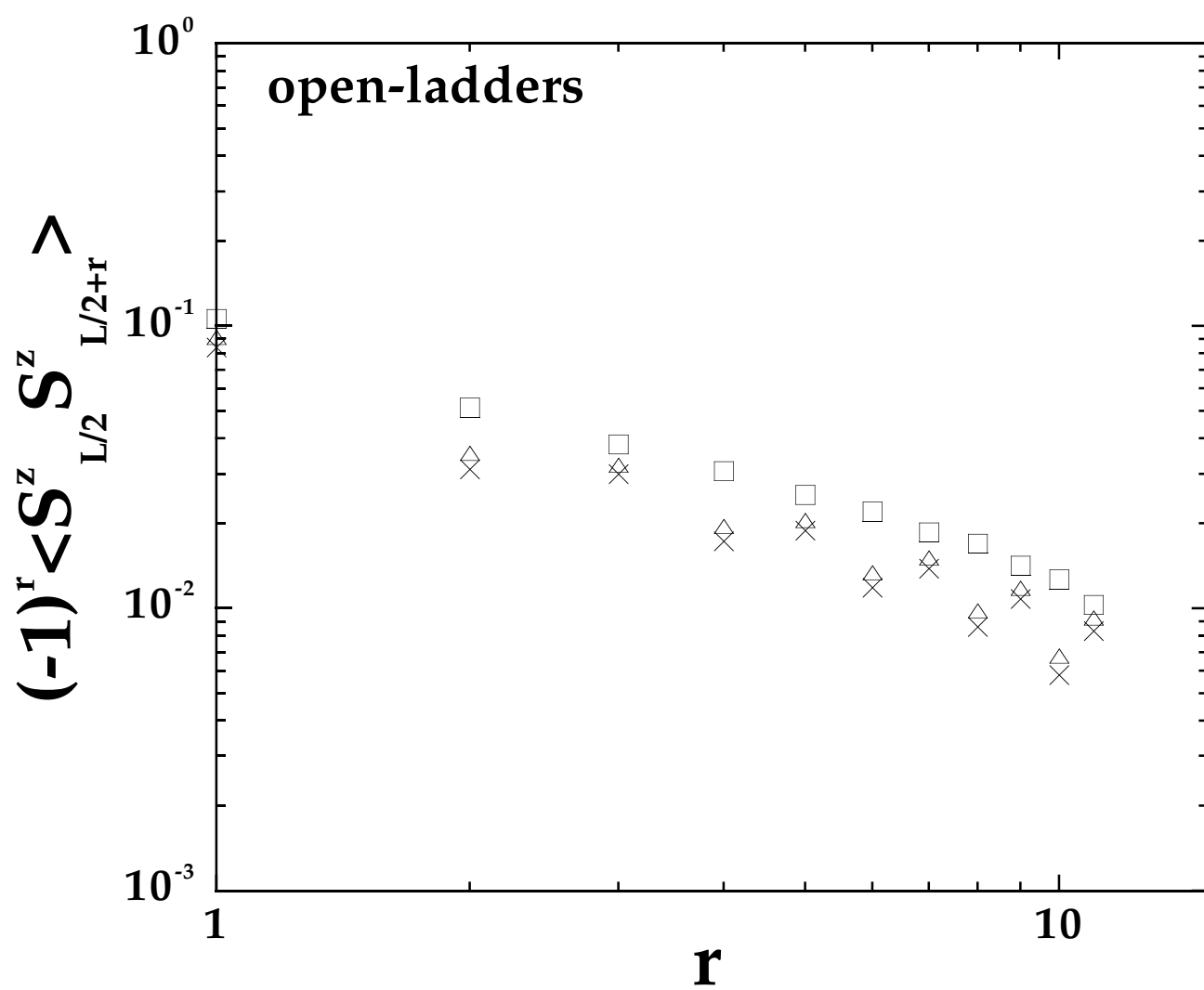


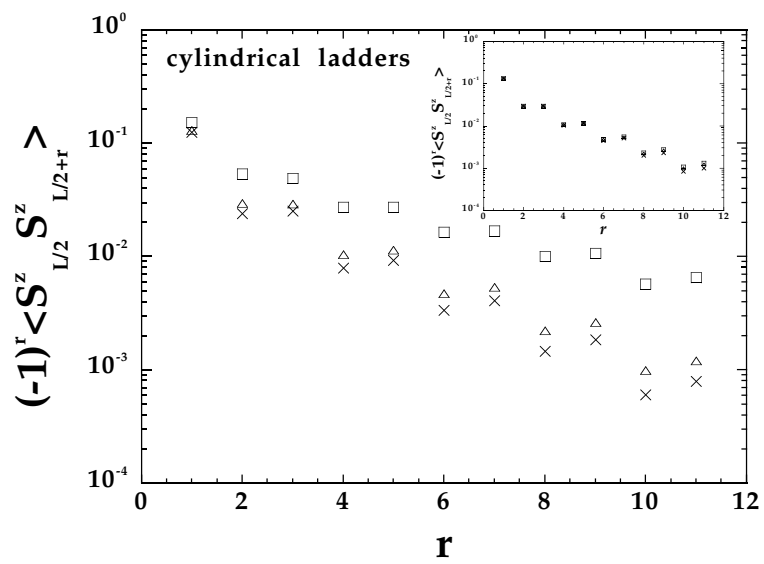


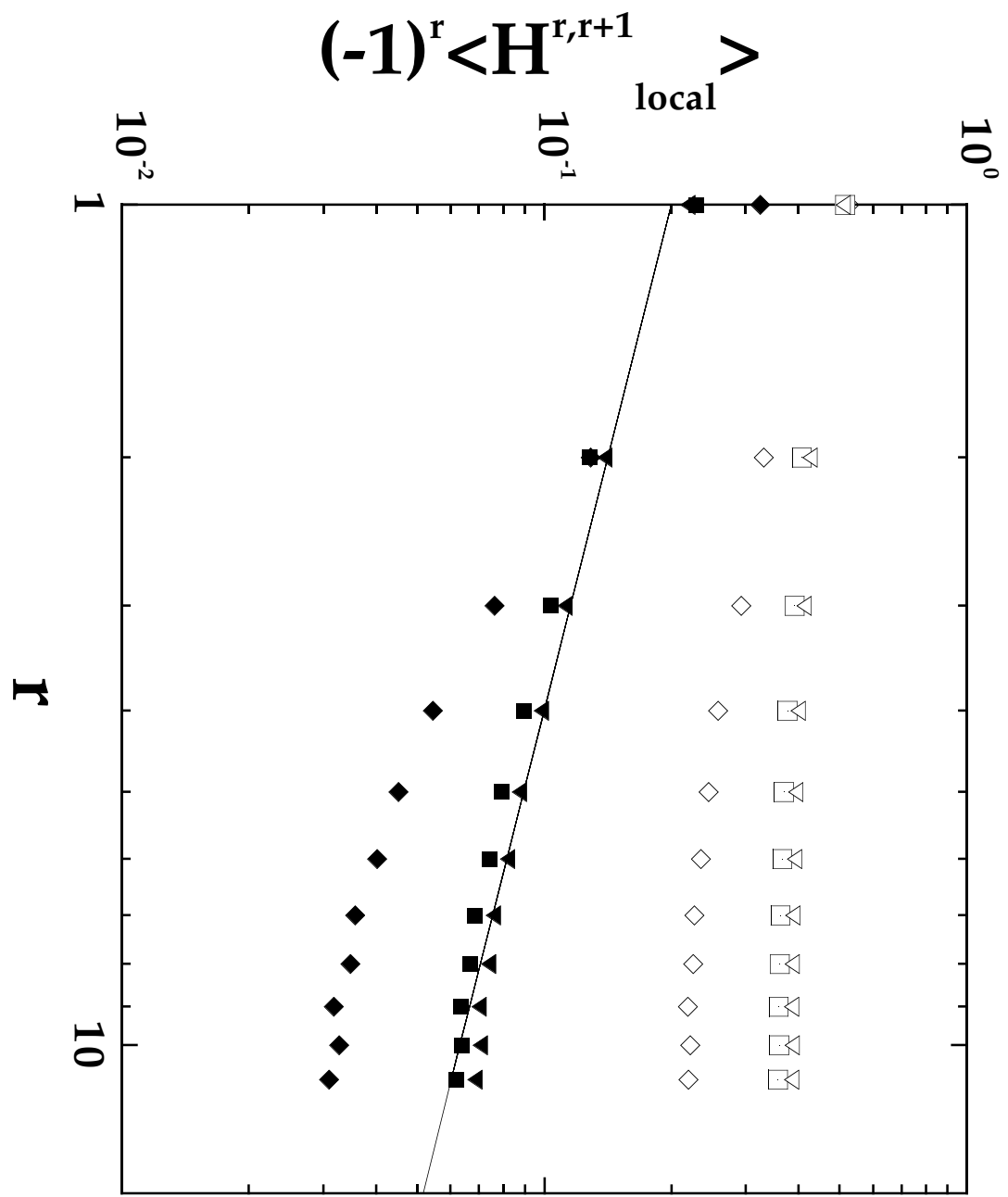


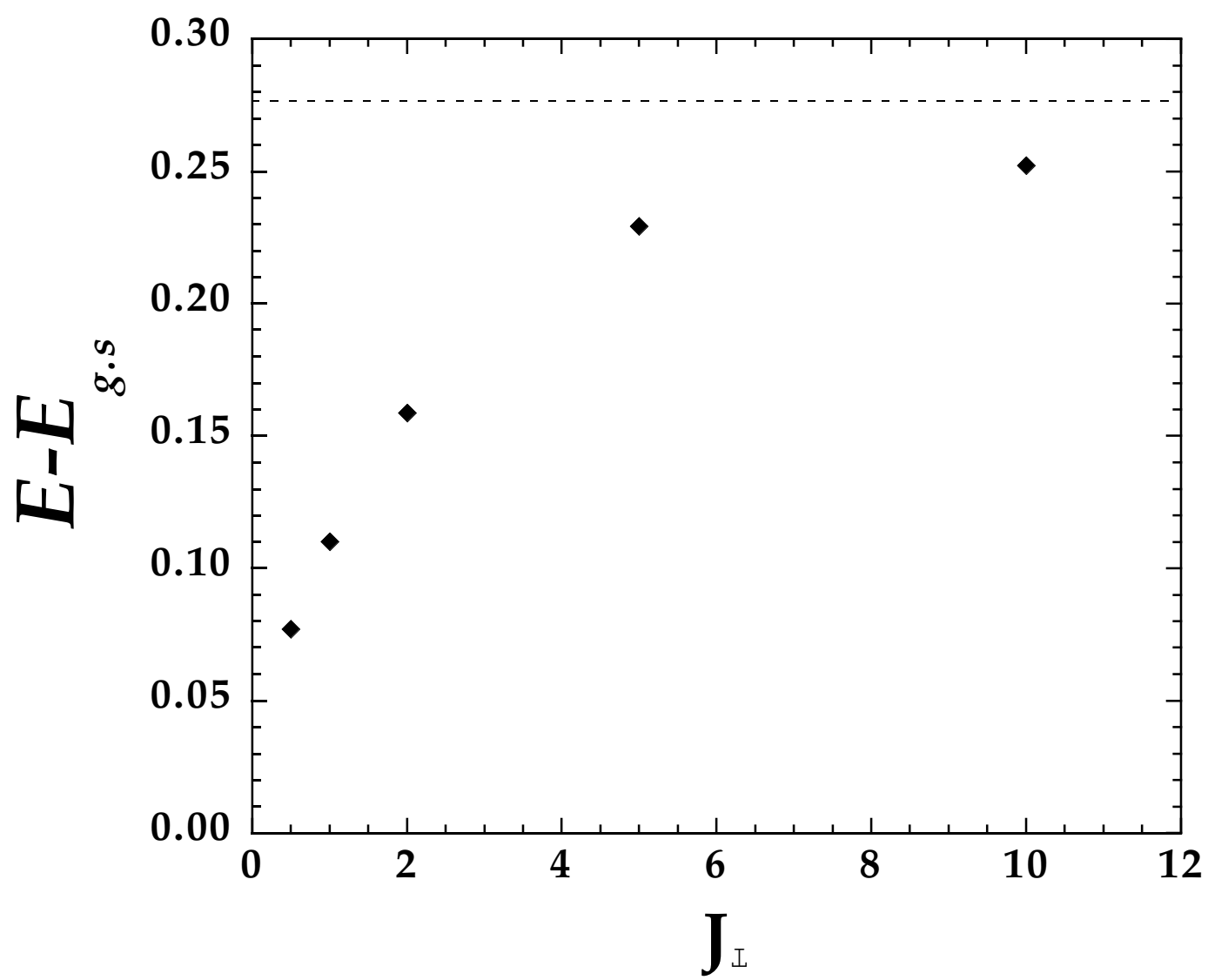


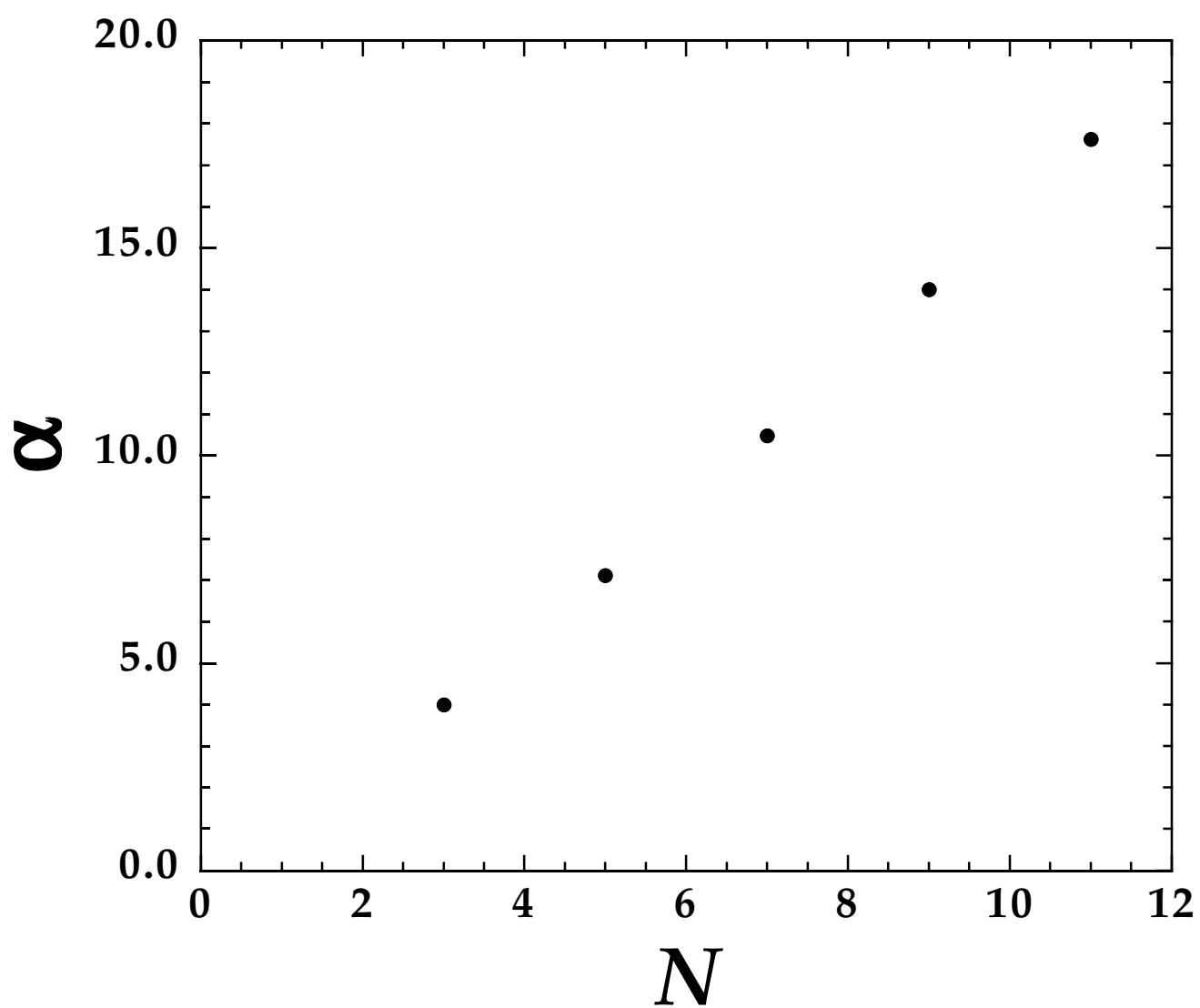


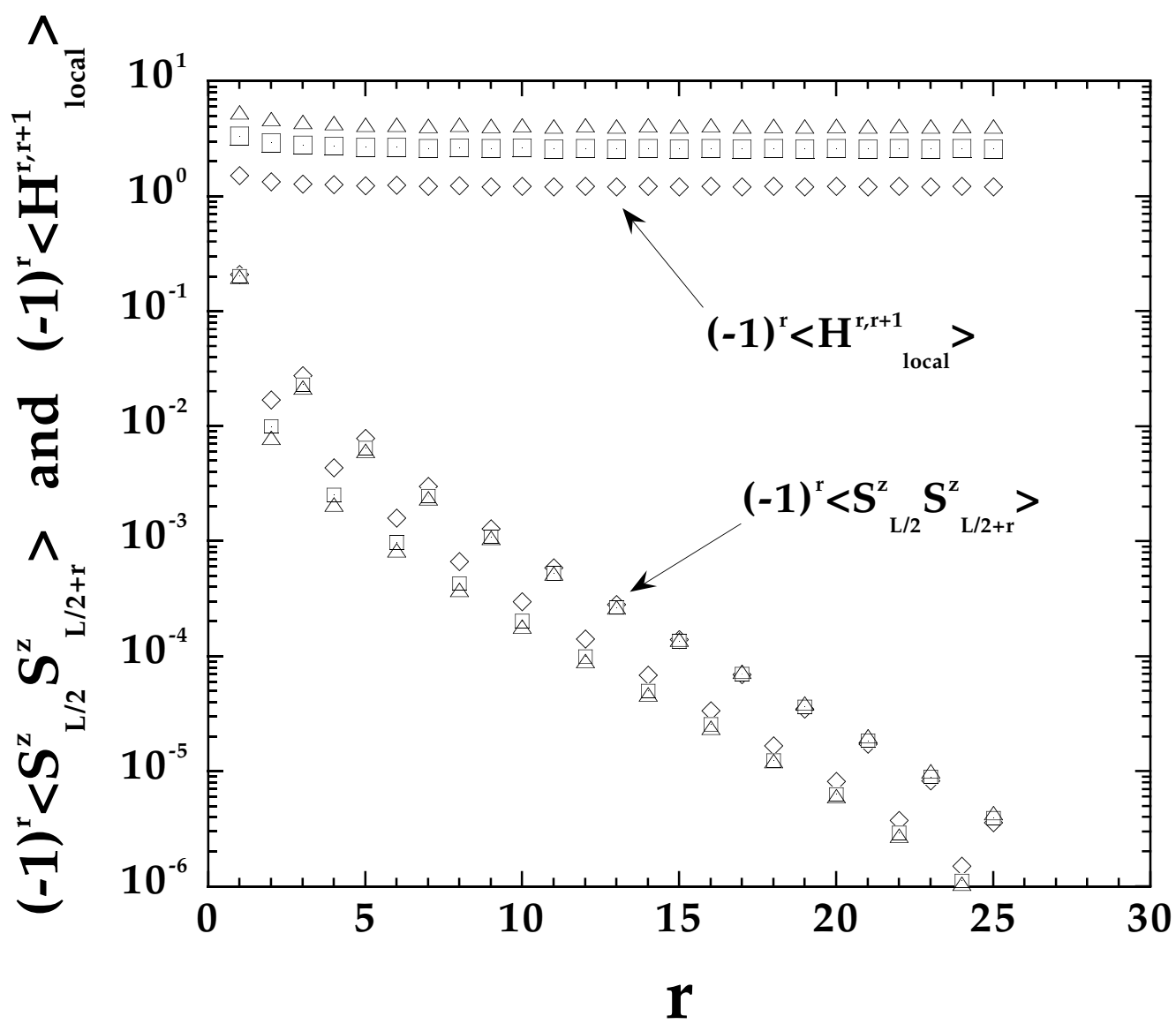


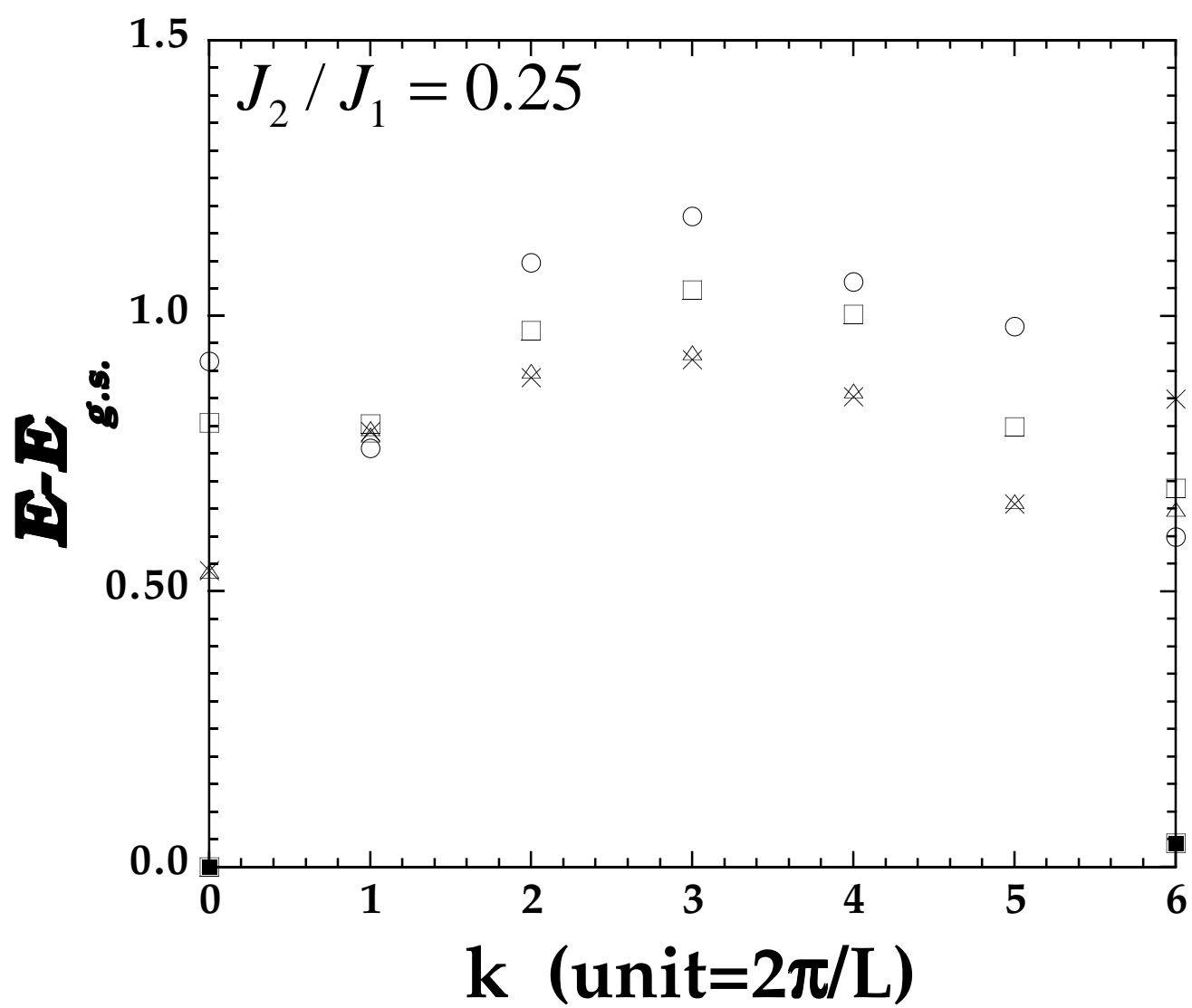


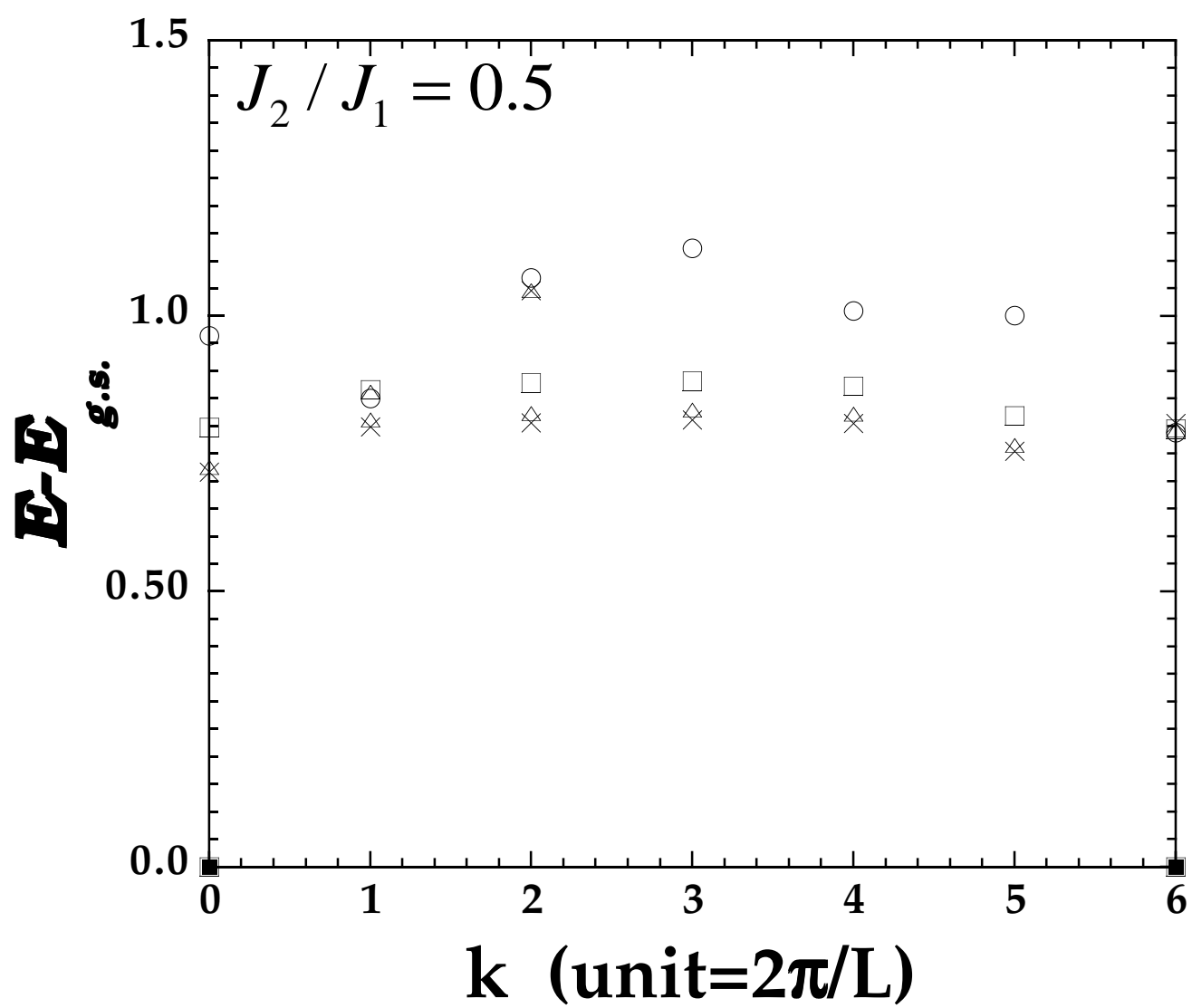












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